The impact of unintentional discrete charges in a nominally undoped channel of a thin body double gate MOSFET: classical to full quantum simulation

A. Martinez[1], J. R. Barker[1], A. Svizhenko[2], M. P. Anantram[2], A. R. Brown[1], B. Biegel[2] and A. Asenov[1]

[1]Nanoelectronics Research Centre, Department of Electronics and Electrical Engineering, University of Glasgow, G12 8LT, Scotland, UK. [2]Nasa Ames Research Center, MS:229-1, Moffett Field, California 94035-1000, USA

jbarker@elec.gla.ac.uk

Abstract. A comparison of full quantum device simulation with semi-classical methods is made for an unintended single atomistic dopant at various locations in a 10 nm double gate MOSFET transistor. The density gradient method comes closest to the non-equilibrium Green function results for fails seriously when the unwanted charge is located well-within the channel.

1. Introduction

The quest for CMOS transistors operating at the nanometre scale has focussed attention on the role of quantum effects especially confinement effects and tunnelling. At the same time intrinsic fluctuations in device characteristics, for example due to discrete dopants, do not average out [1, 2]. In novel, thin body double gate MOSFETs, which do not require channel doping [3], unintentional doping may be introduced during the wafer or device fabrication process. Although low in probability such stray doping, which could introduce significant change in the device characteristics [4, 5], becomes increasingly important bearing in mind the huge count of transistors per chip. Electrons or holes trapped on defect states at the interface or in the gate oxide could have similar effect. Such defect states could also be created by radiation in space applications and could affect the reliability of circuits for space missions. Therefore it becomes increasingly important to be able to resolve the impact of individual discrete charges on the characteristics of nano-CMOS device in numerical device simulations. However, there is a high computational cost in all but the simplest methodologies.

The aim of this work is to compare the capabilities of three of the most commonly used simulation techniques, Drift-Diffusion (DD), Density Gradient (DG) and Non-Equilibrium Green's Functions

1. REPORT DATE **2006**	2. REPORT TYPE **N/A**	3. DATES COVERED **-**	
4. TITLE AND SUBTITLE **The Impact of Unintentional Discrete Charges in a Nominally Undoped Channel of a Thin Body Double Gate MOSFET: Classical to Full Quantum Simulati**		5a. CONTRACT NUMBER	
		5b. GRANT NUMBER	
		5c. PROGRAM ELEMENT NUMBER	
6. AUTHOR(S)		5d. PROJECT NUMBER	
		5e. TASK NUMBER	
		5f. WORK UNIT NUMBER	
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) **Nanoelectronics Research Centre, Department of Electronics and Electrical Engineering, University of Glasgow, G12 8LT, Scotland, UK**		8. PERFORMING ORGANIZATION REPORT NUMBER	
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)		10. SPONSOR/MONITOR'S ACRONYM(S)	
		11. SPONSOR/MONITOR'S REPORT NUMBER(S)	
12. DISTRIBUTION/AVAILABILITY STATEMENT **Approved for public release, distribution unlimited**			
13. SUPPLEMENTARY NOTES **The Seventh International Conference on New Phenomena in Mesoscopic Structures & The Fifth International Conference on Surfaces and Interfaces of Mesoscopic Devices, November 27th - December 2nd, 2005, Maui, Hawaii, USA, The original document contains color images.**			
14. ABSTRACT			
15. SUBJECT TERMS			

16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT **SAR**	18. NUMBER OF PAGES **4**	19a. NAME OF RESPONSIBLE PERSON
a. REPORT **unclassified**	b. ABSTRACT **unclassified**	c. THIS PAGE **unclassified**			

(NEGF) [6], to handle the impact of localised discrete charges on the characteristics of a nano-MOSFETs. Although the microscopic descriptions of transport are different for the different techniques, we will place the emphasis of the comparison the subthreshold regime where the characteristics of the devices are electrostatically dominated and the carrier transport model plays a secondary role [6,7]. It is important to note that in the subthreshold region the DD approach just considers thermionic emission over the potential barrier, but the DG approach captures the carrier confinement and lowers the potential barrier, increasing the thermionic current, effectively mimicking tunnelling to some degree. By comparison NEGF rigorously includes all quantum mechanical effects, such as tunnelling and confinement but omits scattering. The low computational cost of DD and DG (compared to the NEGF method) makes these approaches very attractive for modelling based design and analysis of nano-devices, particularly when the impact of localised charges has to be studied on a statistical scale. Of course the proper treatment of quantum effects associated with localised charges in the channel requires full scale 3D quantum transport simulations. However, a 3D NEGF device simulation is very computationally expensive and an almost intractable task for current computers. For this reason we are restricted to a 2D NEGF simulator and therefore adopt a 2D approach for DD and DG to allow a meaningful comparison with the NEGF formalism. A localised charge in the 2D simulation represents a uniform charged wire running in direction normal to the channel cross section. The sharp potential barrier produced by the wire provides a good basis for comparing the three techniques.

2. Test model

The testbed for our simulations is a 10 nm channel length double gate MOSFET (DGMOSFET), illustrated in Fig. 1, which justifies the use of a ballistic approach used in NEGF technique. In general, the location of the single stray charge in the device is completely random. However, in the case of our 2-dimensional simulations we consider three different key cases of charge location: halfway along the channel in the middle, halfway along the channel at one interface, and at the source-channel junction in the middle of the channel. The channel thickness is 3nm, the doping in the source and drain regions is 10^{20} cm^{-3}, and the background channel doping, is 10^{14} cm^{-3}.
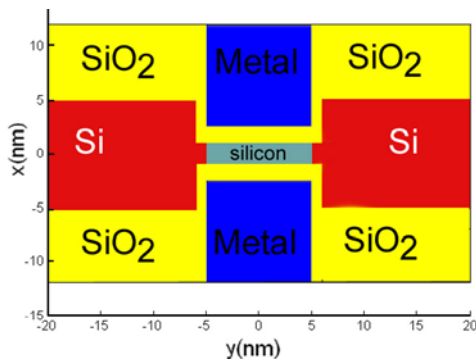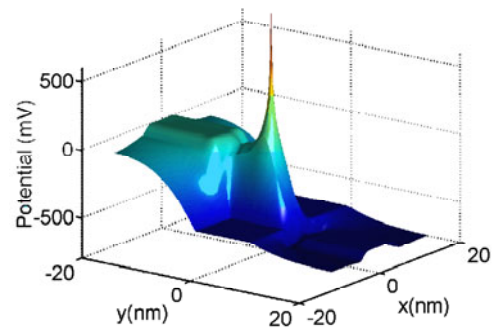

Fig. 1. Structure of the DGMOSFET.

Fig. 2. 2D potential distribution with a charge in the centre of the channel. $V_G = 1.0$V and $V_D = 0.6$V.

The 2D potential profile for the case of a centrally located charge is shown in Fig. 2. Figs. 3 (a) & (b) show the density of states from NEGF simulation along the centre line of the transistor, midway between the two gates, for a gate potential of 1.0 V without and with the fixed charge present, respectively.
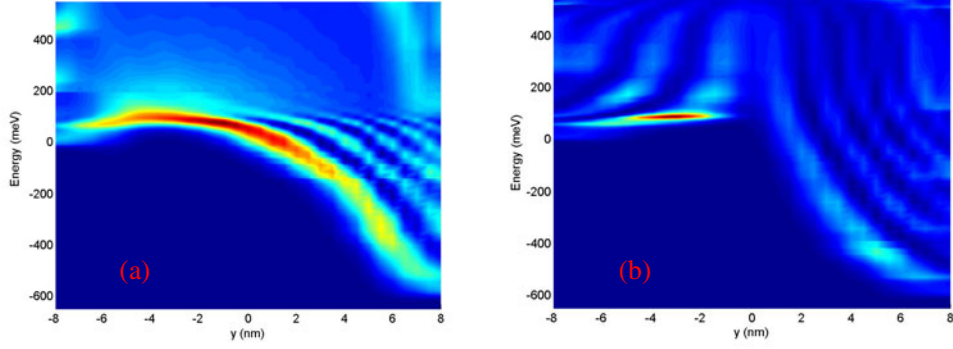
Fig. 3. Density of states through the middle of the channel at V_G = 1V. (a) without stray charge; (b) 1 stray charge placed at the centre of the channel.

3. Results of the simulations

The resulting I_D-V_G characteristics are shown in Fig. 4(a), 4(b) and 4(c) for the three cases respectively comparing the DD, DG and NEGF approaches. The threshold voltage and the shape of the I_D-V_G characteristics are strongly affected by the position of the charge in the channel.
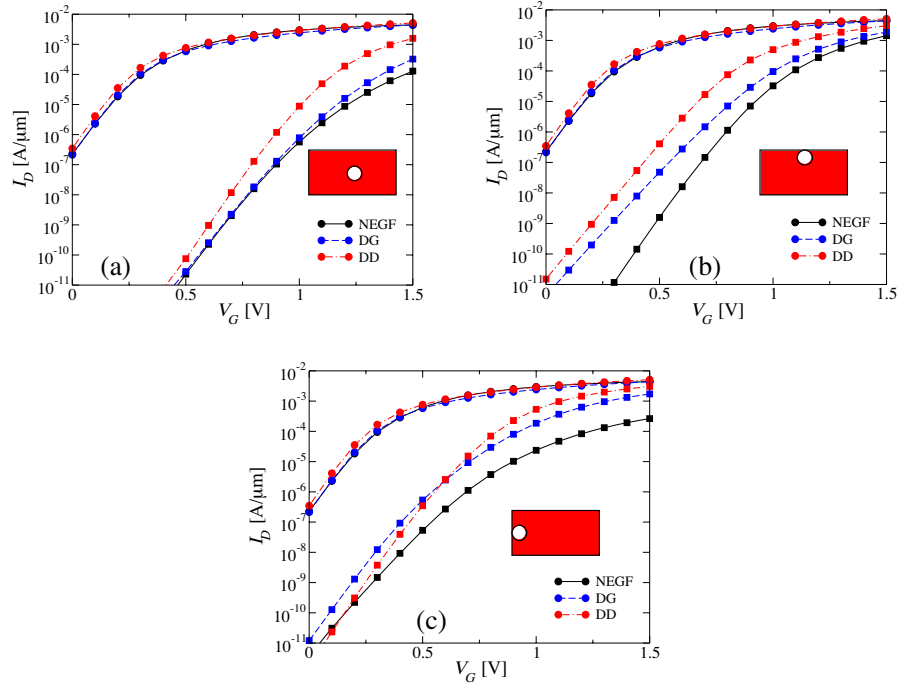

Fig. 4 . I_D-V_G characteristics without a charge (circles) and with a charge located: (a) in the centre of the channel (squares);

(b) halfway along the channel at the interface (squares); (c) at the source-channel junction in the middle (squares).

The electron concentration in a vertical cross-section through the added charge is shown in Fig. 5 for all the cases and approaches. This demonstrates a high penetration of electrons through the potential barrier associated with the charge when NEGF is used, showing that only NEGF completely accounts for tunnelling.
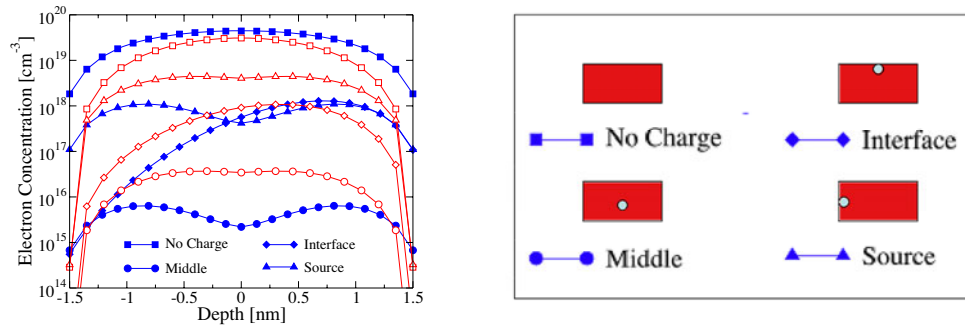
Fig. 5. Electron concentration on a vertical cross-section through the added charge, comparing Density Gradient (filled symbols) with Non equilibrium Green Function simulation (open symbols).

4. Conclusions

It is observed from Fig. 6 that the density gradient is highly successful when there is no channel dopant. The charge offset property which follows from quantum confinement is quite well-replicated. There is close agreement for a charge embedded at the interface. For isolated charges the charge distribution is poorly modeled by density gradient; the situation is worst for a charge in the centre of the channel where significant tunnelling occurs. On the other hand, the current-voltage characteristics are quite well-reproduced by the density gradient method which does provide some barrier lowering thus mimicking tunnelling. The strong deviation of the drift-diffusion and density gradient current-voltage predictions for the other charge locations is associated with micro-vortex formation at different contributing energies[8,9,10]. The situation worsens for discrete dopant clusters (we have studied up to 4) where multiple-scattering and macro-vortices arise. When sufficient impurities are present the wave interference leads to self-averaging but this requires many thousands of dopants. It is observed that the lowest conductance occurs for the channel blocking of Fig. 4(c), as expected.

Acknowledgments

References

[1]   A. Asenov, S. Kaya and A. R. Brown, IEEE Trans. Electron Devices, **50**,1254-1260 (2003).
[2]   A. R. Brown, A. Asenov and J. R. Watling, IEEE Trans. Nanotechnology, **1**, 95-200 (2002).
[3]   Z. Ren, *et al*, IEDM Tech. Digest, 715–718 (2000).
[4]   A. R. Brown, J. R. Watling and A. Asenov, J. Comp. Elec., **1**, 165-169 (2002).
[5]   D. Vasileska and S. S. Ahmed, IEEE Trans. Electron Dev., **52**, 27-236 (2005).
[6]   A. Svizhenko, M. P. Anantram, T. R Govindan and B. Siegel, J. App. Phys. **91**, 2343 (2002).
[7]   A. Asenov, J.R. Watling, A. R. Brown and D. K. Ferry, J. Comp. Elec., **1**, 503-513, (2002).
[8]   J. R. Barker, Microelectronic Engineering, **63**, 223-231 (2002).
[9]   J. R. Barker and A. Martinez, J. Comp. Elec., **3**, 401-405 (2004).
[10]   J.R. Barker, Physica, **E19**, 62-70, (2003).